

## SEARCH REQUEST FORM

## Scientific and Technical Information Center

Requester's Full Name: DAWN GARRETT Examiner #: 76107 Date: 5/20/2003  
 Art Unit: 1774 Phone Number 305-0788 Serial Number: 09/842,228  
 Mail Box and Bldg/Room Location: CP3 11D03 Results Format Preferred (circle): PAPER DISK E-MAIL  
(mailbox) CP3 8B32-Room

If more than one search is submitted, please prioritize searches in order of need.

parent of  
10/173,253

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Filing date 4/26/2001

Title of Invention: ORGANIC LUMINOUS MATERIAL AND ORGANIC

LIGHT-EMITTING DEVICE

Inventors (please provide full names): KOTA YOSHIKAWA, MASASHI KISHIMA,  
HIDEKI SHIRAKAWA, IKUO KINOSHITA

Earliest Priority Filing Date: JAPAN 2000-128364 4/27/00, JP 2000-288692 9/22/00

\*For Sequence Searches Only\* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number. JP 2001-125359 4/4/01

(These compounds are used in an organic light emitting device)  
 Please search formula (1) where benzene is the

aromatic ring, paraphenylenes is the first allylene group (Ar1), metaphenylenes is the second aromatic group (Ar2), alkoxy group is the first, second, third, and forth substituents.

also search where

aromatic groups are benzene and the substituents can be any one of hydrogen, alkyl, alkoxy, carboxyl, cyano, phenyl, biphenyl, or cyclohexylphenyl

<b>STAFF USE ONLY</b>		Type of Search	Vendors and cost where applicable
Searcher:	<u>EL</u>	NA Sequence (#)	STN <u>\$ 367.35</u>
Searcher Phone #:		AA Sequence (#)	Dialog
Searcher Location:		Structure (#)	<u>(6) subsets</u> Questel/Orbit
Date Searcher Picked Up:	<u>5-21-03</u>	Bibliographic	<u>(and)</u> Dr. Link
Date Completed:		Litigation	Lexis/Nexis
Searcher Prep & Review Time:	<u>10</u>	Fulltext	Sequence Systems
Clerical Prep Time:		Patent Family	WWW/Internet
Online Time:	<u>105</u>	Other	Other (specify)

=> file reg

FILE 'REGISTRY' ENTERED AT 12:04:14 ON 21 MAY 2003  
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FILE 'HCAPLUS' ENTERED AT 10:32:26 ON 21 MAY 2003  
L1 17236 S KOTA ?/AU OR YOSHIKAWA ?/AU  
L2 2149 S MASASHI ?/AU OR KIJIMA ?/AU  
L3 3407 S HIDEKI ?/AU OR SHIRAKAWA ?/AU  
L4 15570 S IKUO ?/AU OR KINOSHITA ?/AU  
L5 1 S L1 AND L2 AND L3 AND L4  
SEL L5 1 RN

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L7 3 S L6 AND PMS/CI

FILE 'HCAPLUS' ENTERED AT 10:35:04 ON 21 MAY 2003  
L8 5 S L7

FILE 'LREGISTRY' ENTERED AT 10:35:20 ON 21 MAY 2003  
L9 STR  
L10 STR

FILE 'REGISTRY' ENTERED AT 10:40:15 ON 21 MAY 2003  
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L13 50 S L9 AND L10 AND L11  
L14 STR L9  
L15 STR L10  
L16 50 S L14 AND L15 AND L11  
E POLYACETYLENE/PCT  
L17 10092 S E3  
E POLYOTHER/PCT  
L18 210231 S E3  
E POLYOTHER ONLY/PCT  
L19 69904 S E3  
L20 1724 S L14 AND L15 AND L11 FUL  
SAV L20 GAR228/A  
L21 1437 S L20 AND (L17 OR L19)

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L22 STR

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L28 STR

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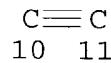
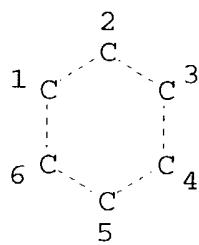
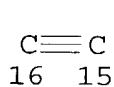
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L37 3 S L34 AND L36  
L38 3 S L35 AND L36  
L39 2 S L8 AND L36  
L40 857 S L21  
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L49 8 S L8 OR L37 OR L38 OR L39  
L50 4 S L48 NOT L49  
L51 16 S L47 NOT (L49 OR L50)  
SEL L51 1-16 HIT RN

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=> d l24 que stat  
L11 SCR 2043  
L14 STR



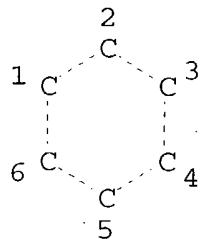
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STEREO ATTRIBUTES: NONE  
 L15 STR



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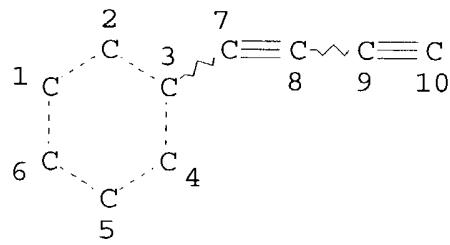
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## STEREO ATTRIBUTES: NONE

L20 1724 SEA FILE=REGISTRY SSS FUL L14 AND L15 AND L11  
 L22 STR



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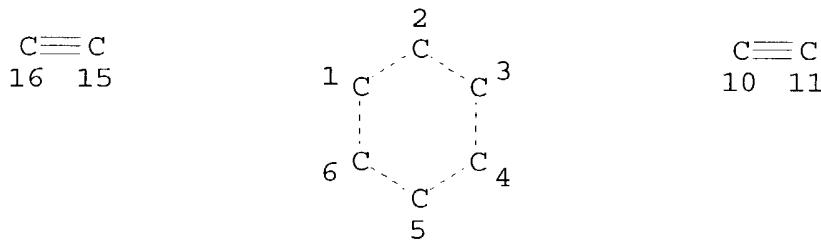
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116 ANSWERS

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 L11 SCR 2043  
 L14 STR



## NODE ATTRIBUTES:

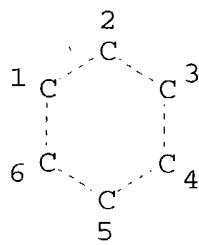
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## GRAPH ATTRIBUTES:

RSPEC I  
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## STEREO ATTRIBUTES: NONE

L15 STR



## NODE ATTRIBUTES:

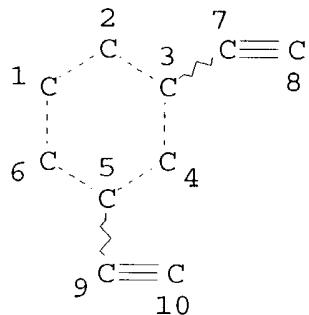
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## GRAPH ATTRIBUTES:

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## STEREO ATTRIBUTES: NONE

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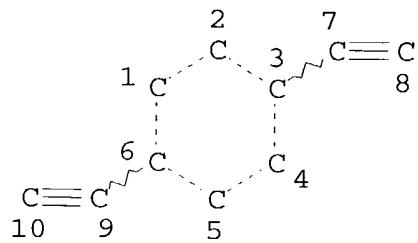
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RSPEC I  
 NUMBER OF NODES IS 10

## STEREO ATTRIBUTES: NONE

L28 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE

L30 92 SEA FILE=REGISTRY SUB=L20 SSS FUL L27 AND L28

100.0% PROCESSED 528 ITERATIONS

92 ANSWERS

SEARCH TIME: 00.00.01

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L49 ANSWER 1 OF 8 HCAPLUS COPYRIGHT 2003 ACS

2002:650752 Document No. 137:311312 Synthesis, Chain Rigidity, and Luminescent Properties of Poly[(1,3-phenyleneethynylene)-alt-tris(2,5-dialkoxy-1,4-phenyleneethynylene)]s. Chu, Qinghui; Pang, Yi; Ding, Liming; Karasz, Frank E. (Department of Chemistry, Center for High Performance Polymers and Composites, Clark Atlanta University, Atlanta, GA, 30314, USA). Macromolecules, 35(20), 7569-7574 (English) 2002. CODEN: MAMOBX. ISSN: 0024-9297. Publisher: American Chemical Society.

AB Sol. poly[(1,3-phenyleneethynylene)-alt-tris(2,5-dialkoxy-1,4-phenyleneethynylene)] derivs. (I) have been synthesized by using the Heck-type coupling reaction. Even with a significant increase in the p-phenyleneethynylene content, the copolymers exhibit a random-coil conformation in THF soln., with a Mark-Houwink exponent detd. to be  $\alpha$ . apprxeq. 0.78. As a result of the extended conjugation length of the chromophore, the absorption and emission

.lambda.max values of I are notably red-shifted (by about 30-40 nm) from that of poly[(1,3-phenyleneethynylene)-alt-(2,5-dialkoxy-1,4-phenyleneethynylene)] derivs. (II). The fluorescence quantum efficiency of I is estd. to be .phi.fl .apprxeq. 0.50, slightly higher than that of II (.phi.fl .apprxeq. 0.44). The fluorescence of I in the solid state is strong, indicating its potential for various device applications. LEDs based on I emitted green-yellow EL with an external quantum efficiency of 0.013%.

IT 472987-13-6P 472987-14-7P 472987-15-8P

472987-16-9P

(synthesis, chain rigidity, and luminescent properties of poly[(1,3-phenyleneethynylene)-alt-tris(2,5-dialkoxy-1,4-phenyleneethynylene)]s)

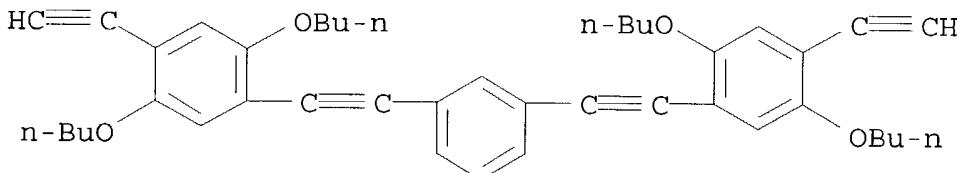
RN 472987-13-6 HCPLUS

CN Benzene, 1,4-dibutoxy-2,5-diido-, polymer with 1,3-bis[(2,5-dibutoxy-4-ethynylphenyl)ethynyl]benzene (9CI) (CA INDEX NAME)

CM 1

CRN 472987-11-4

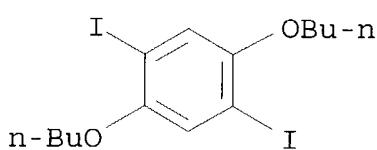
CMF C42 H46 O4



CM 2

CRN 145483-70-1

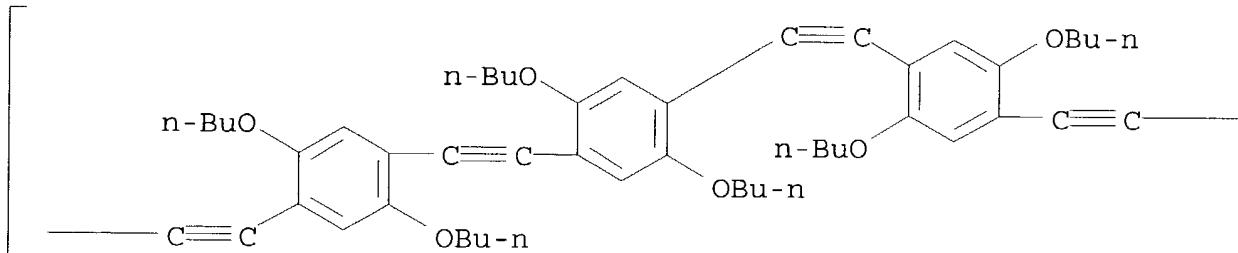
CMF C14 H20 I2 O2



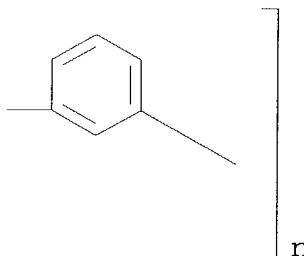
RN 472987-14-7 HCPLUS

CN Poly[1,3-phenylene-1,2-ethynediyl(2,5-dibutoxy-1,4-phenylene)-1,2-ethynediyl(2,5-dibutoxy-1,4-phenylene)-1,2-ethynediyl(2,5-dibutoxy-1,4-phenylene)-1,2-ethynediyl] (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



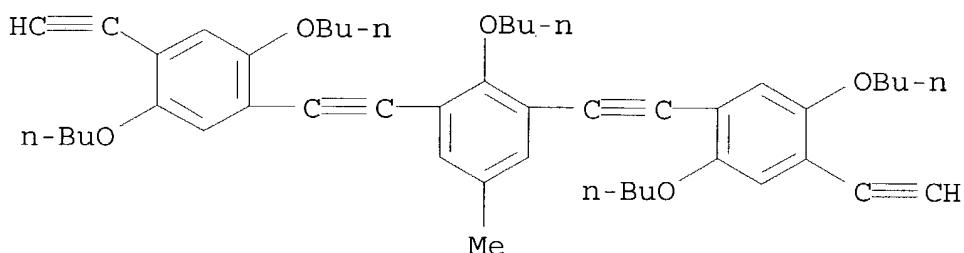
RN 472987-15-8 HCPLUS

CN Benzene, 2-butoxy-1,3-bis[(2,5-dibutoxy-4-ethynylphenyl)ethynyl]-5-methyl-, polymer with 1,4-dibutoxy-2,5-diiodobenzene (9CI) (CA INDEX NAME)

CM 1

CRN 472987-12-5

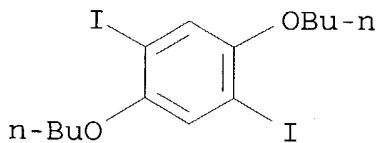
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CRN 145483-70-1

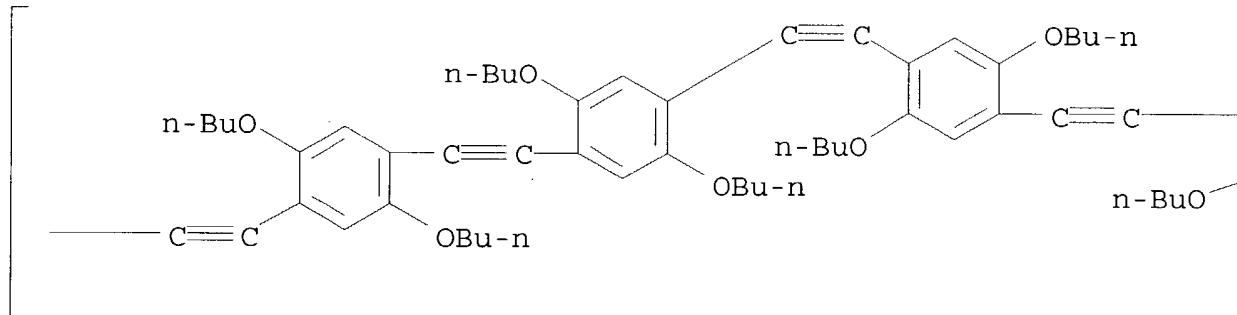
CMF C14 H20 I2 O2



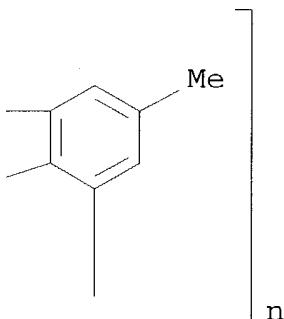
RN 472987-16-9 HCPLUS

CN Poly[(2-butoxy-5-methyl-1,3-phenylene)-1,2-ethynediyl(2,5-dibutoxy-1,4-phenylene)-1,2-ethynediyl(2,5-dibutoxy-1,4-phenylene)-1,2-ethynediyl(2,5-dibutoxy-1,4-phenylene)-1,2-ethynediyl] (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



CC 35-5 (Chemistry of Synthetic High Polymers)

Section cross-reference(s): 73

ST polyphenyleneethynylene deriv synthesis structure luminescence  
optical property; **electroluminescence**  
polyphenyleneethynylene deriv light emitting  
diode

IT **Electroluminescent devices**

(contg. poly[(1,3-phenyleneethynylene)-alt-tris(2,5-dialkoxy-1,4-phenyleneethynylene)]s)

IT Brightening

Electric current-potential relationship

Luminescence, **electroluminescence**

(of **LED** contg. poly[(1,3-phenyleneethynylene)-alt-tris(2,5-dialkoxy-1,4-phenyleneethynylene)]s)

IT 472987-13-6P 472987-14-7P 472987-15-8P

472987-16-9P

(synthesis, chain rigidity, and luminescent properties of poly[(1,3-phenyleneethynylene)-alt-tris(2,5-dialkoxy-1,4-phenyleneethynylene)]s)

L49 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2003 ACS

2002:540528 Document No. 137:248067 Highly luminescent diyne (-C.ident.C-C.ident.C-) containing hybrid polyphenyleneethynylene/poly(p-phenylenevinylene) polymer: synthesis and characterization. Egbe, Daniel Ayuk Mbi; Birckner, Eckhard; Klemm, Elisabeth (Institut fur Organische Chemie und Makromolekulare Chemie der Friedrich-Schiller-Universitat Jena, Jena, D-07743, Germany). Journal of Polymer Science, Part A: Polymer Chemistry, 40(15), 2670-2679 (English) 2002. CODEN: JPACEC. ISSN: 0887-624X. Publisher: John Wiley & Sons, Inc..

AB Luminophoric dialdehyde 1,4-bis[4-formylphenylethynyl-(2,5-dioctadecyloxyphenyl)-buta-1,3-diyne] (I) was used to prep. diyne-contg. hybrid poly(phenylene-ethynylene)/poly(p-phenylene-vinylene)s. Poly[1,4-phenylene-ethynylene-1,4-(2,5-dioctadecyloxy)phenylene-butadi-1,3-ynylene-1,4-(2,5-dioctadecyloxy)phenylene-ethynylene-1,4-phenylene-ethene-1,2-diyl-1,4-(2,5-dioctadecyloxy)phenylene-ethene-1,2-diyl] (II) was obtained, which has a well-defined structure (-Ph-C.ident.C-Ar-C.ident.C-C.ident.C-Ar-C.ident.C-Ph-CH=CH-Ar-CH=CH-)n, as confirmed by NMR and IR spectroscopy. The highly luminescent II material is thermally stable, sol. in common org. solvents due to octadecyloxy side groups, and can be processed into transparent films. The effect of -C.ident.C-C.ident.C- segments on the photophys. response of II was studied and compared to that of monomers [1,4-bis(4-formylphenylethynyl)-2,5-dioctadecyloxybenzene] (III) and I and of their resp. polymers, II and IV (III homopolymer). The polymers showed similar photophys. response in dil. CHCl3 soln. as they have an identical chromophore system responsible for absorption (.lambda.a = 448 nm) and emission (.lambda.f = 490 nm). The increased planarization and enhanced rigidity of the conjugated backbone in the solid state at room temp. and in frozen dil. THF soln. at 77 K cause a bathochromic shift in the absorption and emission spectra. The large octadecyloxy side chains obviously limit strong .pi.-.pi. interchain interactions in the solid films, which explains the high fluorescence quantum yield, 35 and 52%, for IV and II, resp. The energetically arduous migration of .pi. electrons through the diyne units requires a higher threshold voltage for the detection of photocond. in II but could possibly limit radiationless deactivation channels of the exciton, which

explains the approx. 20% fluorescence quantum yield difference between IV and II in the solid state. The electron-withdrawing effect of the triple bonds confer both IV and II with good electron-accepting property ( $E_{ox} = 1.39$  V vs. Ag/AgCl), suitable for use in light-emitting diode devices.

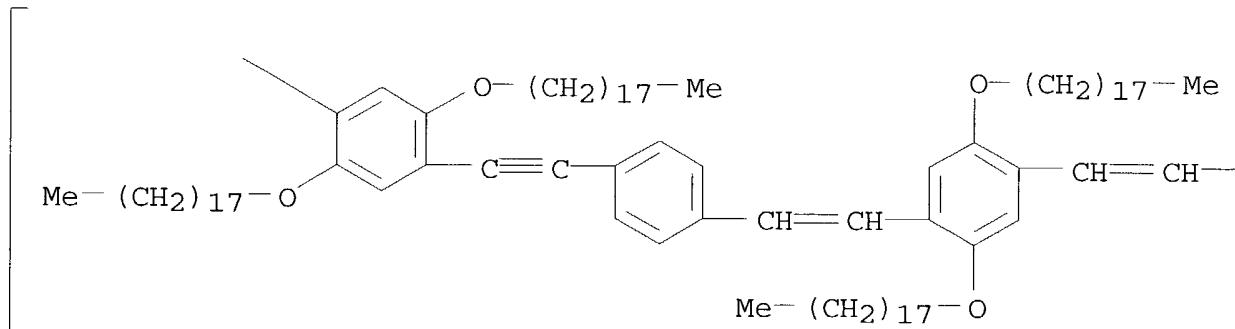
IT 460983-64-6P, 1,4-Bis[4-formylphenylethyynyl-(2,5-dioctadecyloxyphenyl)-buta-1,3-diyne]-2,5-dioctadecyloxy-p-xylylene-bis(diethyl)phosphonate copolymer, SRU

(prepn. of highly luminescent diyne-contg. polyacetylene/poly(p-phenylenevinylene) and role of triple bond segment on chain rigidity and acceptor levels on photocond.)

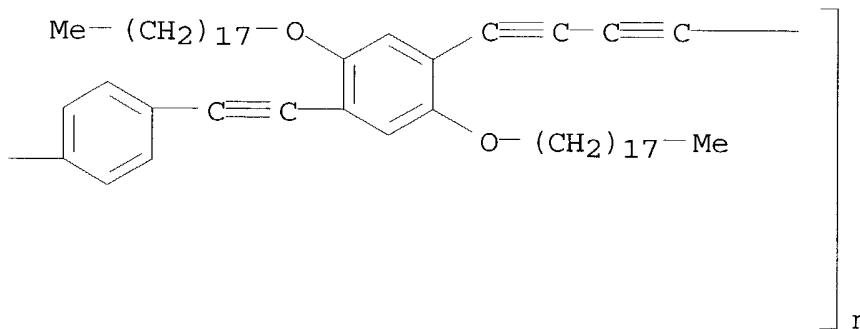
RN 460983-64-6 HCPLUS

CN Poly[[2,5-bis(octadecyloxy)-1,4-phenylene]-1,2-ethynediyl-1,4-phenylene-(1E)-1,2-ethenediyl[2,5-bis(octadecyloxy)-1,4-phenylene]-(1E)-1,2-ethenediyl-1,4-phenylene-1,2-ethynediyl[2,5-bis(octadecyloxy)-1,4-phenylene]-1,3-butadiyne-1,4-diyl] (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



CC 35-7 (Chemistry of Synthetic High Polymers)  
Section cross-reference(s): 36, 73

IT 460983-62-4P, 1,4-Bis[4-formylphenylethyynyl-(2,5-dioctadecyloxyphenyl)-buta-1,3-diyne]-2,5-dioctadecyloxy-p-xylylene-

bis(diethyl)phosphonate copolymer **460983-64-6P**,  
 1,4-Bis[4-formylphenylethynyl-(2,5-dioctadecyloxyphenyl)-buta-1,3-diyne]-2,5-dioctadecyloxy-p-xylylene-bis(diethyl)phosphonate copolymer, SRU

(prepn. of highly luminescent diyne-contg. polyacetylene/poly(p-phenylenevinylene) and role of triple bond segment on chain rigidity and acceptor levels on photocond.)

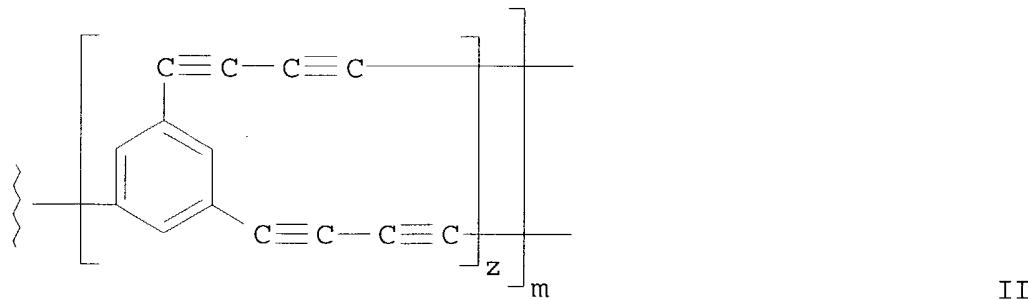
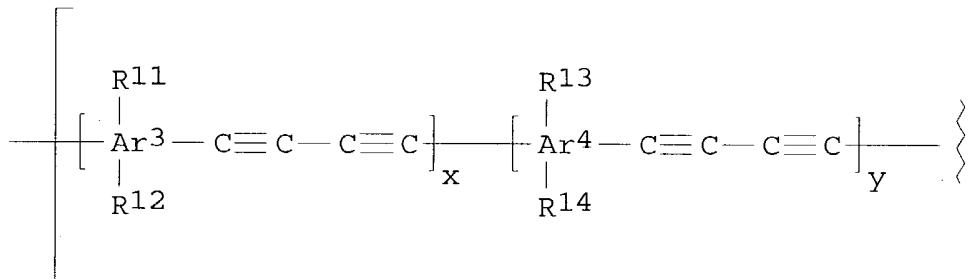
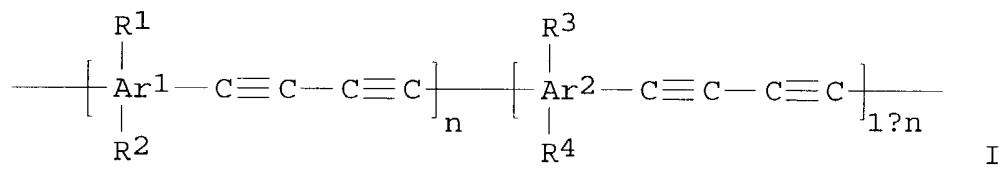
L49 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2003 ACS

2001:868018 Document No. 136:12556 Organic luminescent materials and organic **light-emitting** devices based on them.

Yoshikawa, Kota; Kijima, Masashi; Shirakawa, Hideki; Kinoshita, Ikuo (Fujitsu Limited, Japan). Eur. Pat. Appl. EP 1158839 A2 20011128, 22 pp. DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO. (English). CODEN: EPXXDW. APPLICATION: EP 2001-303861 20010427. PRIORITY: JP 2000-128364 20000427; JP 2000-288692 20000922; JP 2001-125359 20010424.

GI

*Priority documents*



AB Luminescent materials are described by the general formulas I and II (Ar1-4 = arylene groups; R1-4, R11-14 = same or different)

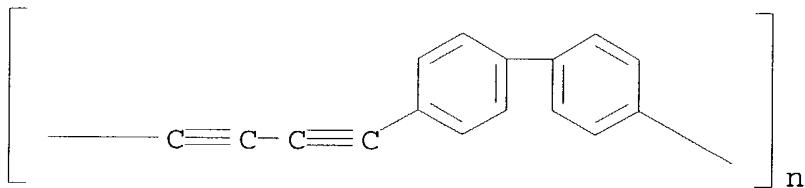
substituents; n,x,y,z = copolymer ratios; and m = d.p.). Thus, green-emitting, red-emitting and blue-emitting luminescent materials were synthesized and characterized. Org. light-emitting devices are also described which comprise a lower electrode; a luminescent layer formed on the lower electrode and made of polymer I or II; and an upper electrode formed on the luminescent layer.

IT 121265-60-9P 375395-26-9P

(blue-emitting; org. luminous materials and org. light-emitting devices based on them)

RN 121265-60-9 HCPLUS

CN Poly([1,1'-biphenyl]-4,4'-diyl-1,3-butadiyne-1,4-diyl) (9CI) (CA INDEX NAME)



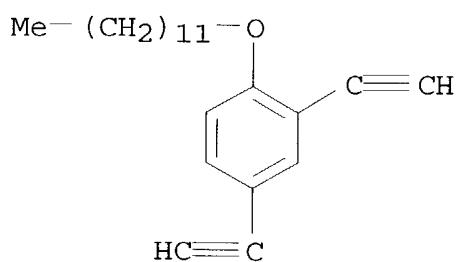
RN 375395-26-9 HCPLUS

CN Benzene, 1,4-bis(dodecyloxy)-2,5-diethynyl-, polymer with 1-(dodecyloxy)-2,4-diethynylbenzene and 1,3,5-triethynylbenzene (9CI) (CA INDEX NAME)

CM 1

CRN 350237-28-4

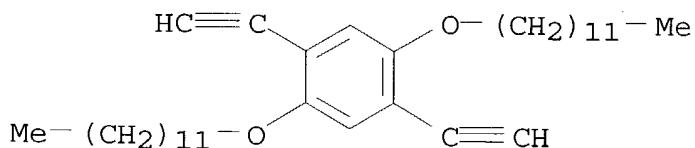
CMF C22 H30 O



CM 2

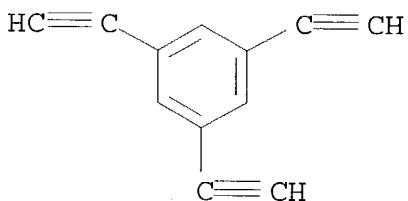
CRN 152270-00-3

CMF C34 H54 O2



CM 3

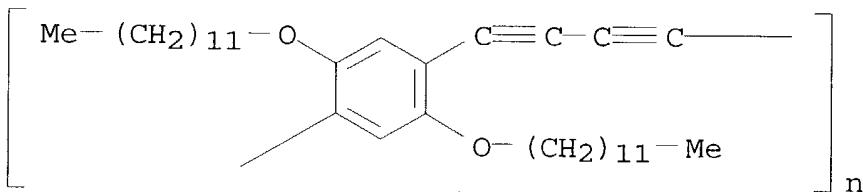
CRN 7567-63-7

CMF C<sub>12</sub> H<sub>6</sub>

IT 227329-08-0P

(green-emitting; **org. luminous** materials and  
**org. light-emitting** devices based on  
them)

RN 227329-08-0 HCPLUS

CN Poly[[2,5-bis(dodecyloxy)-1,4-phenylene]-1,3-butadiyne-1,4-diyl]  
(9CI) (CA INDEX NAME)IC ICM H05B033-14  
ICS C08F038-00

CC 73-5 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)

Section cross-reference(s): 25, 38, 76

ST **org** polymer **luminescent** material **light**  
**emitting** deviceIT Polymers, uses  
(co-; **org.** **luminescent** materials and  
**org.** **light-emitting** devices based on  
them)IT Alkali metals, uses  
Alkaline earth metals

(electrode; **org. luminous** materials and  
**org. light-emitting** devices contg.)

IT **Electroluminescent** devices  
 (org. **luminous** materials and **org.**  
**light-emitting** devices based on them)

IT **Luminescent** substances  
 (**org. luminous** materials prep'd. using)

IT 121265-60-9P 375395-26-9P  
 (blue-emitting; **org. luminous** materials and  
**org. light-emitting** devices based on  
 them)

IT 227329-08-0P  
 (green-emitting; **org. luminous** materials and  
**org. light-emitting** devices based on  
 them)

IT 92-86-4, 4,4'-Dibromobiphenyl 1066-54-2, Trimethylsilylacetylene  
 7567-63-7, 1,3,5-Triethynylbenzene 27342-88-7, Dodecanol  
 50855-13-5, Thiophenecarboxylic acid  
 (**org. luminous** materials prep'd. using)

IT 7311-70-8P 29619-44-1P, 4,4'-Bis(trimethylsilylethylyn) biphenyl  
 38215-38-2P, 4,4'-Diethynylbiphenyl 375395-19-0P 375395-20-3P  
 (**org. luminous** materials prep'd. using)

IT 7440-50-8, Copper, uses  
 (**org. luminous** materials prep'd. using  
 oxidative condensation polymn. catalyzed by)

IT 152270-00-3 350237-28-4  
 (**org. luminous** materials prep'd. using  
 oxidative condensation polymn. of)

L49 ANSWER 4 OF 8 HCPLUS COPYRIGHT 2003 ACS  
 2001:792855 Document No. 136:248147 Anomalous molecular alignment of liquid crystalline conducting conjugated polymer, poly(2,5-dialkoxy-p-phenylenebutadiynylene), using conventional rubbing process. Ozaki, Masanori; Fujisawa, Takeshi; Fujii, Akihiko; Tong, Laga; Yoshino, Katsumi; Kijima, Masashi; Kinoshita, Ikuo; Shirakawa, Hideki (Dep. Electronic Eng., Fac. Eng., Osaka Univ., 2-1 Yamada-oka, Suita, Osaka, 565-0871, Japan). Denki Zairyo Gijutsu Zasshi, 9(2), 192-195 (English) 2000. CODEN: DZGZFE. ISSN: 0918-9890. Publisher: Denki Zairyo Gijutsu Kondankai.

AB The mol. alignment characteristics of liq. cryst. conducting polymer, poly(2,5-dialkoxy-p-phenylenebutadiynylene), were studied. Through a conventional simple rubbing procedure, a uniform mol. alignment with a high quality in a sandwich cell of liq. cryst. conducting polymer, PDAPB, including triple bonds in the main chain was realized by cooling down from the isotrophic phase. An anomalous mol. alignment in which the alkoxy side chain aligned in parallel with the rubbing direction and the mesogenic main chains aligned in perpendicular to the rubbing axis was reported. The viscosity of PDAPB was relatively low compared with the conventional conducting polymers, which was due to flexibility of the conjugated systems in terms of a free rotation of the triple bonds in their main chain. The mol. alignment behavior of the alkoxy side chain of

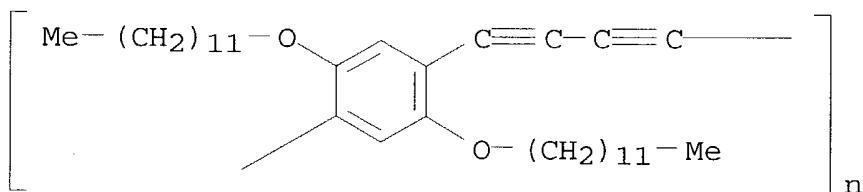
the polymer was quite different from that of a conventional rod-like liq. crystal with low mol. wt. or side-chain type polymeric liq. having a polyacrylate or polysiloxane skeletons.

IT 227329-08-0

(anomalous mol. alignment of liq. cryst. conducting conjugated polymer, poly(2,5-dialkoxy-p-phenylenebutadiynylene), using conventional rubbing process)

RN 227329-08-0 HCPLUS

CN Poly[[2,5-bis(dodecyloxy)-1,4-phenylene]-1,3-butadiyne-1,4-diyl] (9CI) (CA INDEX NAME)



CC 36-5 (Physical Properties of Synthetic High Polymers)  
Section cross-reference(s): 75

IT 227329-05-7 227329-06-8 227329-07-9 227329-08-0

(anomalous mol. alignment of liq. cryst. conducting conjugated polymer, poly(2,5-dialkoxy-p-phenylenebutadiynylene), using conventional rubbing process)

*/cited*

L49 ANSWER 5 OF 8 HCPLUS COPYRIGHT 2003 ACS

1999:265224 Document No. 131:45351 Optical properties of poly(2,5-dialkoxy-p-phenylenebutadiynylene). Fujii, Akihiko; Fujisawa, Takeshi; Yoshino, Katsumi; Kijima, Masashi; Kinoshita, Ikuo; Shirakawa, Hideki (Department of Electronic Engineering, Graduate School of Engineering, Osaka University, Suita, 565-0871, Japan). Japanese Journal of Applied Physics, Part 2: Letters, 38(4A), L406-L409 (English) 1999. CODEN: JAPLD8. ISSN: 0021-4922. Publisher: Japanese Journal of Applied Physics.

AB Optical properties of poly(2,5-dialkoxy-p-phenylenebutadiynylene) (PDAPB), such as optical absorption, photoluminescence (PL) and electroluminescence (EL), have been studied. The electronic energy structures of PDAPB have been detd. by optical and electrochem. measurements. Strong PL with high quantum efficiency has been obsd. in PDAPB, therefore, PDAPB can be considered as a candidate for use in EL materials. Intense EL has been demonstrated in PDAPB for the first time, in conducting polymers with two C-C triple bonds in a unit in the main chain. Anomalous temp. dependence in the absorption spectrum and PL have also been obsd.

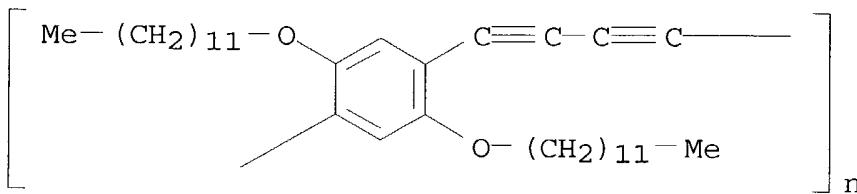
IT 227329-08-0

(216149-55-2; optical properties of poly(2,5-dialkoxy-p-phenylenebutadiynylene))

RN 227329-08-0 HCPLUS

CN Poly[[2,5-bis(dodecyloxy)-1,4-phenylene]-1,3-butadiyne-1,4-diyl]

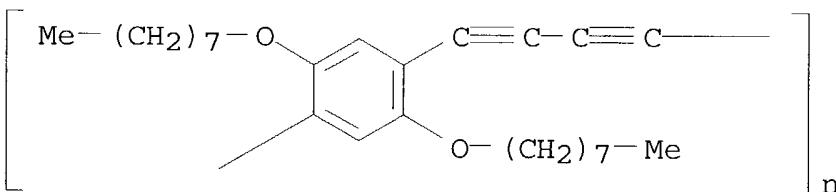
(9CI) (CA INDEX NAME)



IT 227329-06-8

(optical properties of poly(2,5-dialkoxy-p-phenylenebutadiynylene))

RN 227329-06-8 HCPLUS

CN Poly[[2,5-bis(octyloxy)-1,4-phenylene]-1,3-butadiyne-1,4-diyl] (9CI)  
(CA INDEX NAME)CC 36-5 (Physical Properties of Synthetic High Polymers)  
Section cross-reference(s): 73

IT Conducting polymers

Current density

Electric properties

Electronic structure

HOMO (molecular orbital)

LUMO (molecular orbital)

Luminescence

Luminescence, electroluminescence

Optical properties

(optical properties of poly(2,5-dialkoxy-p-phenylenebutadiynylene))

IT 227329-08-0

(216149-55-2; optical properties of poly(2,5-dialkoxy-p-phenylenebutadiynylene))

IT 227329-06-8 227329-07-9

(optical properties of poly(2,5-dialkoxy-p-phenylenebutadiynylene))

L49 ANSWER 6 OF 8 HCPLUS COPYRIGHT 2003 ACS

1998:549014 Document No. 129:246016 A Processible

Poly(phenyleneethynylene) with Strong Photoluminescence: Synthesis and Characterization of Poly[(*m*-phenyleneethynylene)-alt-(*p*-phenyleneethynylene)]. Pang, Yi; Li, Juan; Hu, Bin; Karasz,

Frank E. (Department of Chemistry Center for High Performance Polymers and Composites, Clark Atlanta University, Atlanta, GA, 30314, USA). Macromolecules, 31(19), 6730-6732 (English) 1998. CODEN: MAMOBX. ISSN: 0024-9297. Publisher: American Chemical Society.

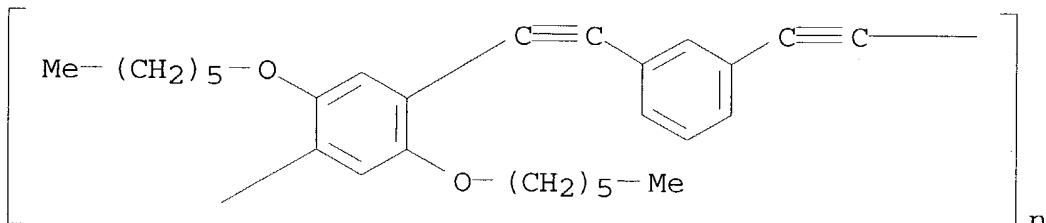
AB The prepn. and characterization of 2,5-bis(hexyloxy)-1,4-diiodobenzene-1,3-diethynylbenzene copolymer is described with respect to development of polyphenyleneacetylenes with improved processability and good luminescent properties. The obsd. monomodal mol. wt. distribution suggested that cyclic products were not formed during the polymn. Incorporation of the m-phenylene unit enabled the chain to effectively adopt a coil-like conformation in soln. Preliminary results indicated that **electroluminescence** could be obtained in a single layer device of the prepd. polymer, although the **EL** spectrum is slightly red-shifted with respect to the photoluminescence spectrum, indicating perhaps the presence of a second electro-optically active species.

IT 213262-79-4P

(prepn. and luminescence of m-phenylene unit-contg. polyphenyleneacetylenes)

RN 213262-79-4 HCPLUS

CN Poly[[2,5-bis(hexyloxy)-1,4-phenylene]-1,2-ethynediyl-1,3-phenylene-1,2-ethynediyl] (9CI) (CA INDEX NAME)



CC 37-5 (Plastics Manufacture and Processing)

Section cross-reference(s): 38, 73

ST processible polyphenyleneethynylene prepn characterization; **electroluminescence** polyphenyleneacetylene; chain conformation polyphenyleneacetylene; luminescence polyphenyleneacetylene chain structure

IT Luminescence

Luminescence, **electroluminescence**

(prepn. and luminescence of m-phenylene unit-contg. polyphenyleneacetylenes)

IT 213262-77-2P 213262-79-4P

(prepn. and luminescence of m-phenylene unit-contg. polyphenyleneacetylenes)

L49 ANSWER 7 OF 8 HCPLUS COPYRIGHT 2003 ACS

1995:584984 Document No. 123:10174 Spectrophotometric determination of phenyl-substituted acetylenes and their polymers in the form of chloranil complexes. Obtemperanskaya, S. I.; Buzlanova, M. M.;

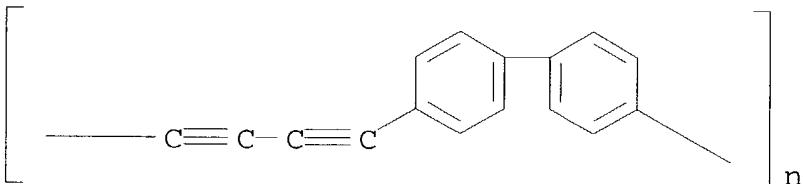
Karandi, I. V.; Shakhid, Rashid; Kashin, A. N. (Moscow State Univ., Moscow, 119899, Russia). Journal of Analytical Chemistry (Translation of Zhurnal Analiticheskoi Khimii), 50(4), 394-6 (English) 1995. CODEN: JACTE2. ISSN: 1061-9348. Publisher: MAIK Nauka/Interperiodica.

AB A spectrophotometric method for detg. Ph-substituted acetylene compds. and their polymers in the form of charge-transfer chloranil (I) complexes permits detn. of the compds. in the range of 10<sup>-7</sup> to 10<sup>-3</sup> M. The Ph-substituted acetylene compds. reacted with I to form colored compds. with a max. of the absorption band in the region of 440 nm.

IT **121265-60-9**  
(spectrophotometric detn. of phenyl-substituted acetylenes and their polymers in form of chloranil complexes)

RN 121265-60-9 HCPLUS

CN Poly([1,1'-biphenyl]-4,4'-diyl-1,3-butadiyne-1,4-diyl) (9CI) (CA INDEX NAME)



CC 35-10 (Chemistry of Synthetic High Polymers)  
Section cross-reference(s): 80

IT 536-74-3, Phenylacetylene 886-66-8, Diphenyldiacetylene  
7223-38-3, Propargyldimethylamine **121265-60-9**

164079-99-6

(spectrophotometric detn. of phenyl-substituted acetylenes and their polymers in form of chloranil complexes)

L49 ANSWER 8 OF 8 HCPLUS COPYRIGHT 2003 ACS

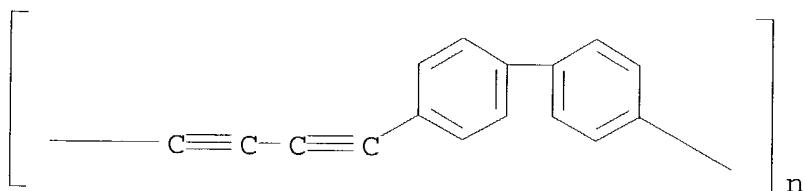
1989:424019 Document No. 111:24019 New rigid-rod monomers and polymers. Wu, Xiaosong; Dirlkov, Stoil K. (Coat. Res. Inst., East. Michigan Univ., Ypsilanti, MI, 48197, USA). Polymeric Materials Science and Engineering, 60, 762-6 (English) 1989. CODEN: PMSEDG. ISSN: 0743-0515.

AB Prepn. of five monomers, HC.tplbond.CRC.tplbond.CH (R = p-phenylene, 2,5-dimethyl-p-phenylene, tetrafluoro-p-phenylene, 4,4'-biphenylene, and octafluoro-4,4'-biphenylene), and polymn. by Glaser coupling to form rigid-rod polymers with triple-bond linkages are reported. The d.p. is estd. to be >20 and most of the polymer remains in soln. There is no difference between the IR spectra of sol. and insol. fractions of the polymers, indicating that no crosslinking has taken place in the insol. fraction.

IT **121265-60-9P**  
(prepn. of, by Glaser coupling of diacetylenic monomer)

RN 121265-60-9 HCPLUS

CN Poly([1,1'-biphenyl]-4,4'-diyl-1,3-butadiyne-1,4-diyl) (9CI) (CA  
INDEX NAME)



CC 35-5 (Chemistry of Synthetic High Polymers)  
IT 28729-99-9P 121265-59-6P **121265-60-9P** 121265-61-0P  
121281-09-2P  
(prepn. of, by Glaser coupling of diacetylenic monomer)

=> d 150 4 hitind

L50 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2003 ACS  
IC ICM C08G061-00  
CC 73-5 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)  
Section cross-reference(s): 35, 38  
IT Dehydrohalogenation  
Heat-resistant materials  
Luminescent substances  
(**light-emitting** material contg.  
phenylene-ethynylene-xylylene polymer and its prepn. by  
dehydrohalogenation coupling reaction)  
IT 110-89-4, Piperidine, uses 1335-23-5, Copper iodide 14221-01-3,  
Tetrakis(triphenylphosphine)palladium  
(dehydrohalogenation catalyst; **light-emitting**  
material contg. phenylene-ethynylene-xylylene polymer and its  
prepn. by dehydrohalogenation coupling reaction)  
IT **122483-16-3P** 160888-96-0P  
(**light-emitting** material contg.  
phenylene-ethynylene-xylylene polymer and its prepn. by  
dehydrohalogenation coupling reaction)

=> d 150 1-4 cbib abs hitstr hitind

L50 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2003 ACS  
2000:539774 Document No. 133:120845 Luminescent group-containing  
diacetylene-based polymers and their use in  
**electroluminescence** devices. Kim, Chung Up; Cho, Hyung Nam;  
Kim, Tong Yong; Kim, Young Chul; Hon, Jae Min; Kim, Jai Kyong; Yu,  
Je Ung (Korea Institute of Science and Technology, S. Korea; Hanfa  
Chemical Corp.). Jpn. Tokkyo Koho JP 3046814 B1 20000529, 18 pp.  
(Japanese). CODEN: JTXXFF. APPLICATION: JP 1999-45846 19990224.

PRIORITY: KR 1999-1056 19990115.

AB The polymers are made from diacetylene compds. which have groups derived from fluorene, 2,7-di(hydroxyphenylethenyl)fluorene, 2,7-di(hydroxyphenyl)fluorene, 1,4-di(hydroxyphenylethenyl)benzene, 1,4-di(hydroxyphenyl)benzene, 3,6-di(hydroxyphenylethenyl)carbazole, or their substituted analogs. **Electroluminescence** devices can be made from a blend of the polymers and other polymers. Thus, bubbling O<sub>2</sub> gas to a mixt. of 2,7-diethynyl-9,9-di-n-hexylfluorene 1.52, CuCl 0.10 and N,N,N',N'-tetramethylethylenediamine 1.50 g in 20 mL chlorobenzene at room temp. for 1 h, pptg. the resulting viscous product with 2.0N HCl and working up gave a polymer.

IT **285143-01-3P 285143-03-5P**

(luminescent group-contg. diacetylene-based polymers and use in **electroluminescence** devices)

RN 285143-01-3 HCPLUS

CN Benzene, 1,4-bis(hexyloxy)-2,5-bis[2-[4-(2-propynyloxy)phenyl]ethenyl]-, homopolymer (9CI) (CA INDEX NAME)

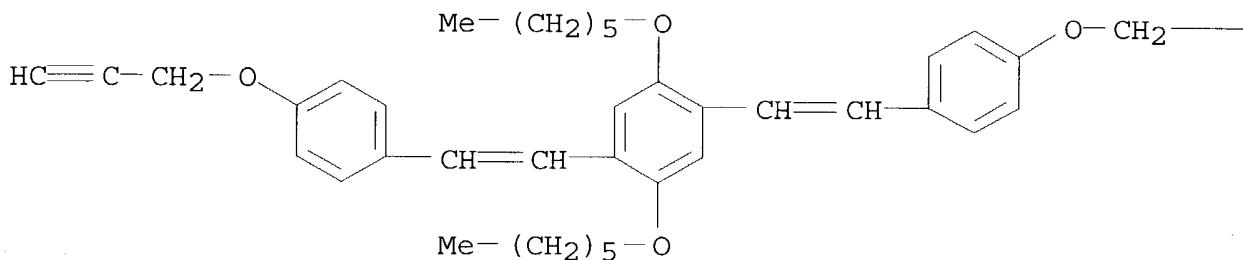
CM 1

CRN 285142-98-5

CMF C40 H46 O4

②

PAGE 1-A



PAGE 1-B

— C≡C CH

RN 285143-03-5 HCPLUS

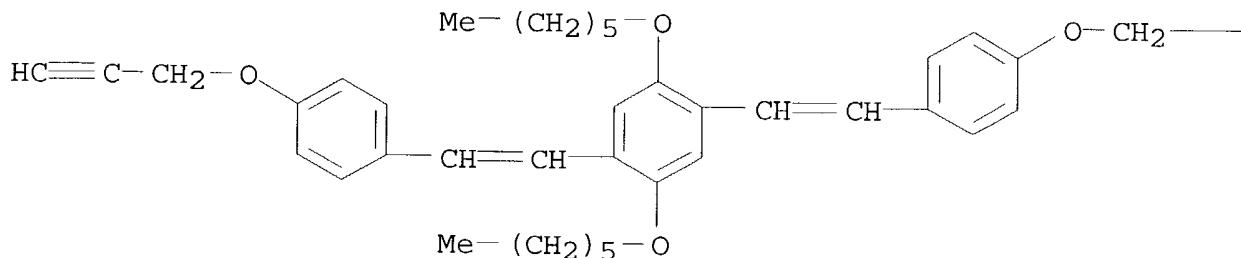
CN 9H-Fluorene, 9,9-dihexyl-2,7-bis[2-[4-(2-propynyloxy)phenyl]ethenyl]-, polymer with 1,4-bis(hexyloxy)-2,5-bis[2-[4-(2-propynyloxy)phenyl]ethenyl]benzene (9CI) (CA INDEX NAME)

CM 1

CRN 285142-98-5

CMF C40 H46 O4

PAGE 1-A



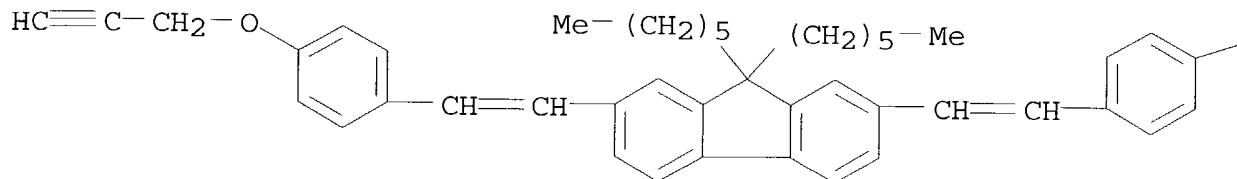
PAGE 1-B

 $-\text{C}\equiv\text{CH}$ 

CM 2

CRN 285142-96-3  
CMF C47 H50 O2

PAGE 1-A



PAGE 1-B

 $-\text{O}-\text{CH}_2-\text{C}\equiv\text{CH}$ 

- IC ICM C08F038-02  
ICS C09K011-06; H05B033-14; C09B069-10  
CC 35-7 (Chemistry of Synthetic High Polymers)  
Section cross-reference(s): 76  
ST luminescent diethynylfluorene polymer **electroluminescence**  
device manuf  
IT **Electroluminescent** devices  
(luminescent group-contg. diacetylene-based polymers and use in  
**electroluminescence** devices)  
IT Polymer blends  
(luminescent group-contg. diacetylene-based polymers and use in

electroluminescence devices)

IT 182500-36-3P 220625-89-8P 270252-32-9P 285142-92-9P  
 285142-93-0P 285142-94-1P 285142-95-2P  
 (intermediate; luminescent group-contg. diacetylene-based polymers and use in **electroluminescence** devices)

IT 285143-05-7P  
 (luminescent group-contg. diacetylene-based polymers and use in **electroluminescence** devices)

IT 285142-99-6P 285143-00-2P **285143-01-3P** 285143-02-4P  
**285143-03-5P** 285143-04-6P  
 (luminescent group-contg. diacetylene-based polymers and use in **electroluminescence** devices)

IT 220625-90-1P 285142-96-3P 285142-98-5P  
 (monomer; luminescent group-contg. diacetylene-based polymers and use in **electroluminescence** devices)

IT 285142-97-4P  
 (reactant; luminescent group-contg. diacetylene-based polymers and use in **electroluminescence** devices)

IT 106-96-7, Propargyl bromide 1066-54-2, Trimethylsilylacetylene 128424-36-2 150623-72-6 189367-54-2  
 (reactant; luminescent group-contg. diacetylene-based polymers and use in **electroluminescence** devices)

L50 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2003 ACS  
 1999:596955 Document No. 131:235518 Boron-containing .pi.-conjugated polymer and **light-emitting** material and nonlinear optical material containing the polymer. Nakajo, Yoshiki; Naka, Kensuke; Matsumi, Noriyoshi (TDK Electronics Co., Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 11255902 A2 **19990921** Heisei, 22 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1998-80193 19980312.

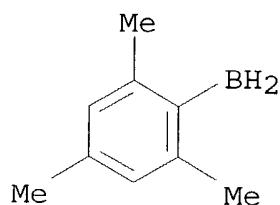
AB The B-contg. .pi.-conjugated polymer is that prep'd. by hydroboration polymn. of monoallylboranes and arom. diyns. The **light-emitting** material and the nonlinear optical material contains the polymer and the materials show improved environment resistance.

IT **207924-53-6P 207924-56-9P**  
 (boron-contg. .pi.-conjugated polymer prep'd. by hydroboration polymn. of monoarylboranes and arom. diyns for **light-emitting** material and nonlinear optical material)

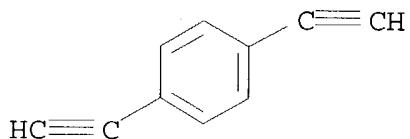
RN 207924-53-6 HCAPLUS  
 CN Borane, (2,4,6-trimethylphenyl)-, polymer with 1,4-diethynylbenzene (9CI) (CA INDEX NAME)

CM 1

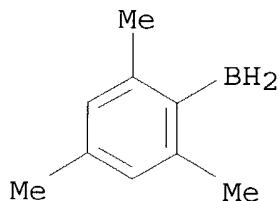
CRN 45741-00-2  
 CMF C9 H13 B



CM 2

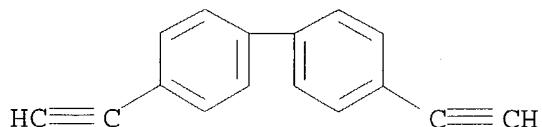
CRN 935-14-8  
CMF C10 H6RN 207924-56-9 HCPLUS  
CN Borane, (2,4,6-trimethylphenyl)-, polymer with 4,4'-diethynyl-1,1'-biphenyl (9CI) (CA INDEX NAME)

CM 1

CRN 45741-00-2  
CMF C9 H13 B

CM 2

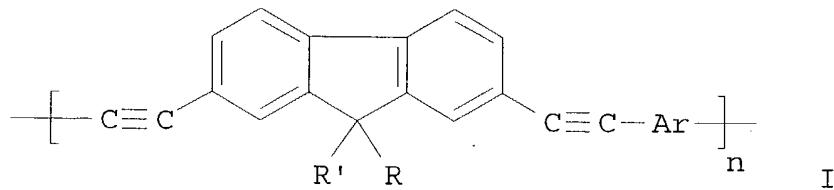
CRN 38215-38-2  
CMF C16 H10



- IC ICM C08G079-08  
ICS C09K011-06; G02F001-35  
CC 73-10 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)  
Section cross-reference(s): 35, 38  
ST boron contg pi conjugated polymer; hydroboration polymn monoarylborane arom diyn; **light emitting**  
material pi conjugated polymer; nonlinear optical material pie conjugated polymer; environment resistance nonlinear optical material  
IT Nonlinear optical materials  
(boron-contg. .pi.-conjugated polymer prep'd. by hydroboration polymn. of monoarylboranes and arom. diyns for **light-emitting** material and nonlinear optical material)  
IT Phosphors  
(**electroluminescent**; boron-contg. .pi.-conjugated polymer prep'd. by hydroboration polymn. of monoarylboranes and arom. diyns for **light-emitting** material and nonlinear optical material)  
IT Polymerization  
(hydroboration; boron-contg. .pi.-conjugated polymer prep'd. by hydroboration polymn. of monoarylboranes and arom. diyns for **light-emitting** material and nonlinear optical material)  
IT Hydroboration  
(polymn.; boron-contg. .pi.-conjugated polymer prep'd. by hydroboration polymn. of monoarylboranes and arom. diyns for **light-emitting** material and nonlinear optical material)  
IT 207924-53-6P 207924-54-7P 207924-56-9P  
207924-57-0P 207924-58-1P 207924-59-2P 207924-60-5P  
207924-61-6P  
(boron-contg. .pi.-conjugated polymer prep'd. by hydroboration polymn. of monoarylboranes and arom. diyns for **light-emitting** material and nonlinear optical material)  
IT 935-14-8P 18512-55-5P 38215-38-2P 45741-00-2P, Mesitylborane  
94463-11-3P  
(monomer; boron-contg. .pi.-conjugated polymer prep'd. by hydroboration polymn. of monoarylboranes and arom. diyns for **light-emitting** material and nonlinear optical material)

element using the same. Kim, Chung Yup; Cho, Hyun Nam; Kim, Dong Young; Kim, Young Chul; Lee, Jun Young; Kim, Jai Kyeong (Korea Institute of Science and Technology, S. Korea). U.S. US 5876864 A 19990302, 27 pp. (English). CODEN: USXXAM. APPLICATION: US 1997-991753 19971216. PRIORITY: KR 1996-82444 19961231.

GI



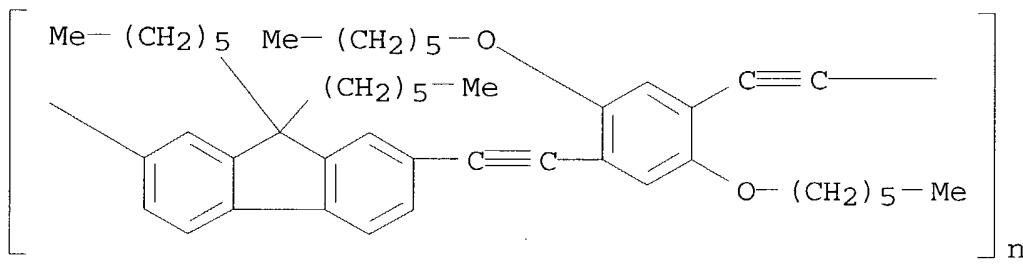
AB **Electroluminescent** polymers are described by the general formula I (R and R' = groups independently selected from H, C1-22 aliph. or alicyclic alkyl or alkoxy groups or C6-18 aryl or aryloxy groups such as Me, Et, Pr, iso-Pr, Bu, iso-Bu, pentyl, hexyl, ethylhexyl, heptyl, octyl, iso-octyl, nonyl, decyl, dodecyl, hexadecyl, octadecyl, cyclopropyl, cyclopentyl, cyclohexyl, methoxy, ethoxy, butoxy, hexyloxy, methoxyethoxyethyl, methoxyethoxyethoxyethyl, Ph, phenoxy, tolyl, benzyl, naphthyl and anthracene groups, alkyl or aryl derivs. of Si, Sn, or Ge such as trimethylsilyl, triphenylsilyl, tributyltin, or triethylgermanium; Ar = Ph, which may be substituted with C1-22 aliph. or alicyclic alkyl or alkoxy groups, di-Ph, diphenylether, diphenylsulfide, diphenylamine, fluorene, terphenyl, naphthalene, anthracene, phenanthrene, heterocyclic compds. such as pyridine, furan, thiophene, alkylthiophene, dithiophene, pyrrole, dipyrrole, dipyrromethane, dibenzofuran, dibenzothiophene, diphenyloxadiazole, diphenylthiadiazole, carbazole, diphenylmethane, diphenylsilane, bisformylphenoxyalkane and isomers or derivs. thereof; and n = an integer > or = 1). **Electroluminescent** devices employing the polymers, optionally in blends with other polymers, are also described.

IT 220625-96-7P 220626-06-2P

(**electroluminescent** acetylene group-contg.  
fluorene-based alternating polymers and  
**electroluminescent** devices using them)

RN 220625-96-7 HCPLUS

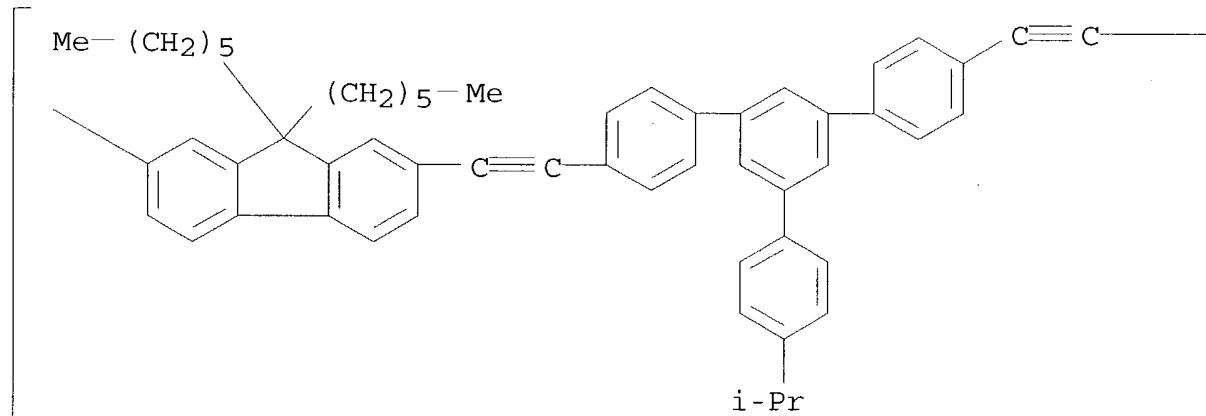
CN Poly[(9,9-dihexyl-9H-fluorene-2,7-diyl)-1,2-ethynediyl[2,5-bis(hexyloxy)-1,4-phenylene]-1,2-ethynediyl] (9CI) (CA INDEX NAME)



RN 220626-06-2 HCAPLUS

CN Poly[(9,9-dihexyl-9H-fluorene-2,7-diyl)-1,2-ethynediyl[5'-[4-(1-methylethyl)phenyl][1,1':3',1'''-terphenyl]-4,4'''-diyl]-1,2-ethynediyl] (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

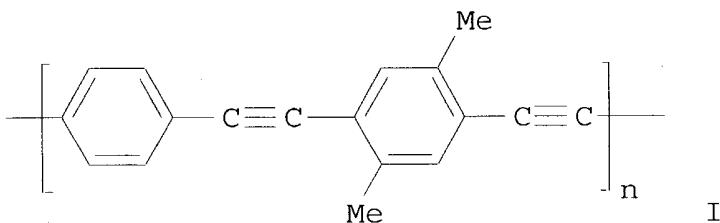
n

IC ICM H05B033-00  
NCL 428690000  
CC 73-11 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)  
Section cross-reference(s): 38, 76  
ST **electroluminescent** fluorene based alternating polymer;  
device **electroluminescent** fluorene based alternating polymer  
IT **Electroluminescent** devices  
(**electroluminescent** acetylene group-contg.  
fluorene-based alternating polymers and  
**electroluminescent** devices using them)  
IT Polyacetylenes, uses  
(**electroluminescent** acetylene group-contg.  
fluorene-based alternating polymers and  
**electroluminescent** devices using them)  
IT Epoxy resins, uses  
(**electroluminescent** acetylene group-contg.  
fluorene-based alternating polymers and  
**electroluminescent** devices using them)  
IT Phosphors  
(**electroluminescent**, polymeric;  
**electroluminescent** acetylene group-contg. fluorene-based  
alternating polymers and **electroluminescent** devices  
using them)  
IT 9003-53-6 9011-14-7, Polymethyl methacrylate 25067-59-8,  
Polyvinylcarbazole  
(**electroluminescent** acetylene group-contg.  
fluorene-based alternating polymers and  
**electroluminescent** devices using them)  
IT 220625-91-2P 220625-92-3P 220625-93-4P 220625-94-5P  
220625-95-6P **220625-96-7P** 220625-97-8P 220625-98-9P  
220625-99-0P 220626-00-6P 220626-01-7P 220626-02-8P  
220626-03-9P 220626-04-0P 220626-05-1P **220626-06-2P**

- (electroluminescent acetylene group-contg.  
fluorene-based alternating polymers and  
**electroluminescent** devices using them)
- IT 189367-54-2P 220625-89-8P 220625-90-1P  
(electroluminescent acetylene group-contg.  
fluorene-based alternating polymers and  
**electroluminescent** devices using them)
- IT 92-86-4, 4,4'-Dibromobiphenyl 106-37-6, 1,4-Dibromobenzene  
108-36-1, 1,3-Dibromobenzene 108-86-1, Bromobenzene, reactions  
523-27-3, 9,10-Dibromoanthracene 591-50-4, Iodobenzene 624-38-4,  
1,4-Diodobenzene 626-39-1, 1,3,5-Tribromobenzene 1066-54-2,  
Trimethylsilyl acetylene 2050-47-7, 4,4'-Dibromodiphenylether  
3001-15-8, 4,4'-Diodobiphenyl 3141-27-3, 2,5-Di-bromothiophene  
7511-49-1 7789-23-3, Potassium fluoride 10016-52-1,  
2,8-Dibromodibenzofuran 31574-87-5, 2,8-Dibromodibenzothiophene  
32460-00-7, 2,5-Dibromofuran 40307-15-1, 2,8-  
Dibromodibenzothiophene-5,5-dioxide 123863-97-8 128424-36-2  
136453-55-9  
(electroluminescent acetylene group-contg.  
fluorene-based alternating polymers and  
**electroluminescent** devices using them)

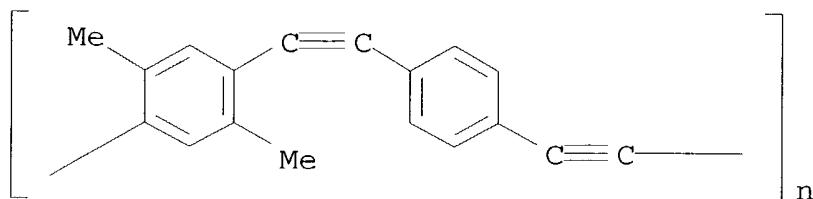
L50 ANSWER 4 OF 4 HCPLUS COPYRIGHT 2003 ACS  
1995:347400 Document No. 122:146661 Linear phenylene-ethynylene-  
xylylene-ethynylene polymer, its preparation, and its-containing  
**light-emitting** material. Yamamoto, Ryuichi;  
Takagi, Masakazu (Yamamoto Ryuichi, Japan; Tatsuta Densen Kk). Jpn.  
Kokai Tokkyo Koho JP 06322077 A2 19941122 Heisei, 5 pp.  
(Japanese). CODEN: JKXXAF. APPLICATION: JP 1993-113279 19930514.

GI



- AB The polymer I is prep'd. by dehydrohalogenation coupling reaction of XArX with HC.tplbond.CAr1C.tplbond.CH (X = halo; Ar, Ar1 = 2,5-xylene-1,4-diyl, 1,4-C6H4; Ar .noteq. Ar1) in the presence of a Pd-Cu catalyst and an amine. The material consists of I. The material showed good heat resistance and chem. stability.
- IT 122483-16-3P  
(**light-emitting** material contg.  
phenylene-ethynylene-xylylene polymer and its prep'n. by  
dehydrohalogenation coupling reaction)
- RN 122483-16-3 HCPLUS

CN Poly[(2,5-dimethyl-1,4-phenylene)-1,2-ethynediyl-1,4-phenylene-1,2-ethynediyl] (9CI) (CA INDEX NAME)



IC ICM C08G061-00  
 CC 73-5 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)

IT Dehydrohalogenation  
 Heat-resistant materials  
 Luminescent substances

(**light-emitting** material contg.  
 phenylene-ethynylene-xylylene polymer and its prepn. by  
 dehydrohalogenation coupling reaction)

IT 110-89-4, Piperidine, uses 1335-23-5, Copper iodide 14221-01-3,  
 Tetrakis(triphenylphosphine)palladium  
 (dehydrohalogenation catalyst; **light-emitting**  
 material contg. phenylene-ethynylene-xylylene polymer and its  
 prepn. by dehydrohalogenation coupling reaction)

IT **122483-16-3P** 160888-96-0P  
 (**light-emitting** material contg.  
 phenylene-ethynylene-xylylene polymer and its prepn. by  
 dehydrohalogenation coupling reaction)